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MODELING OF THE ELASTIC ELECTRONIC POLARIZATION OF FIANITE

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A method of modeling the elastic electronic polarization of fianite is examined. The results of simulation modeling of the long-wavelength optical spectra of zirconium dioxide and yttrium oxide, which are components of this artificial mineral, are presented.

Key words: electronic polarization, electronic orbitals, optical spectrum, modeling efficacy.

Owing to its unique combination of physical and chemical properties fianite is an extremely promising multifunctional material. For example, it is used in the fabrication of optical lenses that can operate at high temperatures as well as withstand chemically aggressive media. Transparent zirconium dioxide crystals with cubic structure (fianite) can be obtained for certain concentrations of the stabilizing oxide, for which yttrium oxide, whose molar concentration can range from 10 to 33%, is used.

It is well known that the elastic electronic polarization of matter is an additive physical property of any dielectric and does not depend on the structure or aggregate state of the dielectric. The minimum time constant of such phenomena occurring when a dielectric interacts with a low-amplitude ac electric field makes it possible to separate their contribution to the total polarized state of a particular object. Thus, effective mathematical modeling of the spectral characteristics of the elastic electronic polarization of zirconium dioxide and yttrium oxide could be very helpful for determining the optimal concentration of the stabilizing oxide in the fabrication of artificial fianite crystals.

It is shown in [1 – 3] that the best mathematical description of the processes under consideration is a model of forced oscillations of the set of all orbitals of separate particle pairs comprising the material of interest. In addition, it was shown that the screening contribution σ^* of the outer electronic orbitals of the oxygen anions is a variable quantity [4]. The values cannot be optimized without using arrays of control values of the optical refractive index $n(\lambda)$ of the sample, measured in the visible range of the optical spectrum. In turn, in practical applications the computational technique used by the authors makes it possible to perform effective simulation modeling of the long-wavelength optical spectra of single crystals of zirconium dioxide ZrO_2 and yttrium oxide Y_2O_3 as well as 12% fianite $ZrO_2 \cdot Y_2O_3$.

The following initial data were used to model the long-wavelength spectrum of the optical refractive index of zirconium dioxide: the physical density $\rho = 5680$ kg/m^3 [5] and the control optical spectrum $n(\lambda)$ in the visible and near-UV ranges [6].

The most effective correspondence between the modeled characteristics of the array of control points, whose plots are shown in Fig. 1, obtains for σ^* values 0.57, 0.50, 0.45 and 0.41 for the $3s^2$, $3p^2$, $3p^4$ and $3p^6$ orbitals of the anion O^{2-}, respectively.

The following initial data were used to model the long-wavelength spectrum of the optical refractive index of yt-

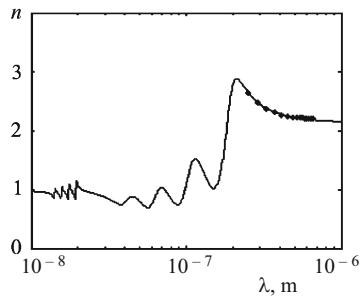

Fig. 1. Optical spectrum of a zirconium dioxide single crystal. The points correspond to the data obtained in a physical experiment.

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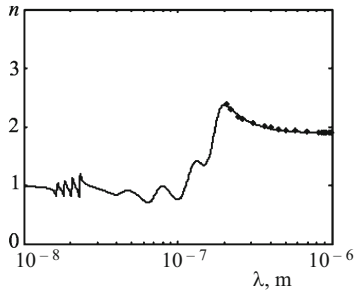

Fig. 2. Optical spectrum of an yttrium oxide single crystal. The points correspond to the data obtained in a physical experiment.

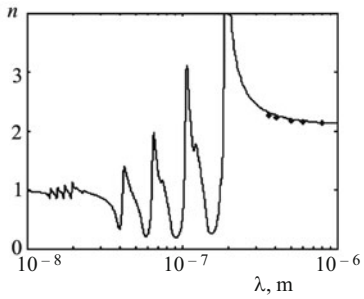

Fig. 3. Optical spectrum of fianite with 12% yttrium oxide content. The points correspond to the data obtained in a physical experiment.

trium oxide: the physical density $\rho = 4850$ kg/m^3 [5] and the control optical spectrum $n(\lambda)$ in the visible and near-UV ranges [6].

The best correspondence between the modeled characteristics of the array of control points, whose plots are shown in Fig. 2, obtains for σ^* values 0.68, 0.55, 0.35 and 0.20 for the $3s^2$, $3p^2$, $3p^4$ and $3p^6$ orbitals of the oxygen anion, respectively.

The control array from [7] was used to model the long-wavelength spectrum of the optical refractive index of fianite with 12% content of yttrium oxide. The optimized values used for the screening contributions of the optical electrons of the oxygen anion were presented above for pure ZrO_2 and Y_2O_3 crystals.

The results of the simulation are presented in Fig. 3.

A general analysis of the correspondence of the simulation spectra of all experimental samples to the data obtained from physical measurements shows unequivocally that the mathematical model used for the electronic polarization is very effective. Therefore, it can be used to reliably predict the optical properties of fianites with different compositions, which, in turn, will make it possible to optimize the technological processes of growing fianites.

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